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Most Significant Accomplishment

This effort produced a fully coupled physical, chemical, biological, and optical numerical model, which at its foundation is the community physical model ROMS 2.2. This physical model enjoys wide spread support in the open source ocean modeling community, and continues to receive development funding from the Navy and the National Science Foundation. The chemical and biological model includes the ability to simulate multiple groups of phytoplankton, multiple limiting nutrients, spectral light harvesting by phytoplankton, multiple particulate and dissolved degradational pools of organic material, and non-stoichometric carbon, nitrogen, phosphorus, silica, and iron dynamics. It also includes a complete spectral light model for the prediction of Inherent Optical Properties (IOPs). The coupling of the predicted IOP model (Ecosim 2.0) with robust radiative transfer model (Ecolight 4.1) was also accomplished, which allows for the direct simulation of remote sensing reflectance. This provides a mechanism by where the physical and ecological model may be directly validated on radiometry rather than an approximation of biomass. The EcoSim 2.0 code has been open-sourced and is part of the distributed ROMS code (http://marine.rutgers.edu/po/models/roms/).

Predicting Upwelling Radiance on the West Florida Shelf

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LONG-TERM GOALS

The prediction of inherent optical properties [IOPs] and water-leaving radiance [L_w] in coastal waters over a 5 to 10 day time horizon will require a numerical simulation that accurately forecasts the physical, ecological, and optical environment. Critical to the ecological and optical forecast is the ability to directly compare the water-leaving radiance field to those being collected by aircraft and satellite platforms. Our goal is to develop the ecological and optical models and computer codes to initialize, validate, and predict the IOPs and L_w over an operational time horizon.

OBJECTIVES

1) Couple EcoSim 2.0 to a robust radiative transfer model to yield water-leaving radiance for a given IOP distribution

2) Initialize and validate spectral water-leaving radiance with remote sensing data.

3) Couple EcoSim 2.0 to the Regional Ocean Modeling System (ROMS)

APPROACH

The pace of development of prognostic ecological/optical data and modeling systems has greatly accelerated in recent years such that we can now reasonably discuss the likelihood of predicting red tides, and concomitant impacts on water clarity on the West Florida Shelf (WFS). Accurate prediction of water clarity and color suggests a fundamental knowledge of marine ecological systems, and the validation of such data and modeling systems would provide characterization of the littoral environment over operational time horizons. Water clarity and color are directly dependent on the IOPs of the water column and the modeling component of these prognostic systems requires a fundamental set of equations that describe the interactions between the production and destruction of the IOPs. As the IOPs of absorption, scattering, and the scattering phase function can be described by a summation of the individual components, the cycle of color can be described by equations representing the individual active color constituents, i.e., phytoplankton, organic detritus, Colored Dissolved Organic Matter (CDOM), sediments, bathymetry, and bottom classification. The description of the

cycling of each component allows for feedback effects between the in-water light field and the production and destruction of color.

The marine optical environment may change at the same time scale of weather change, so any operational prognostic optical system would need to be embedded into a larger system of data collection and numerical modeling. Such a system would use moorings, ships, Autonomous Underwater Vehicles (AUVs), satellites, and physical/ecological/optical numerical models to provide integrated data streams to a wide community of users. The systems would need to be able to assimilate data as it became available, and provide forecasts over a wide range of time and space scales. The West Florida Shelf (WFS) is an ideal location to help develop these nowcast/forecast systems, in part due to a large number of other research programs focused on the WFS, including other ONR funded technology programs, NOAA/EPA ECOlogy of Harmful Algal Blooms (ECOHAB) program, and the State of Florida Coastal Ocean Monitoring and Prediction System (COMPS) program. The ECOHAB and COMPS programs are focused on time scales ranging from months to years and spatial scales ranging from kilometers to 1000s of kilometers. Therefore, this site provides a natural location to develop broad scale time and space models of the inherent optical properties.

The WFS is unique in other ways that make it ideal for the development of forecasting systems. In particular, the variance in color and clarity of the near-shore waters is extreme, ranging from oligotrophic Case 1-type waters to highly attenuating Case 2 waters (Bissett et al., 1997; Carder and Steward, 1985; Carder et al., 1989). The low-nutrient and low-colored waters of the WFS are derived from the oligotrophic waters of the central Gulf of Mexico and the waters of the Caribbean Sea via the Loop Current. These waters have typical open ocean color signals. In the deeper waters off the shelf, the variations in surface color are driven by seasonal nutrients and CDOM introductions via deep mixing, as well as eddy fluxes, much like the classic understanding of Case 1 ocean color. As one moves across the shelf break onto the outer shelf, complications to the classic blue ocean signal arise from both Loop Current intrusions that bring higher nutrient waters (and CDOM) into the euphotic zone and river CDOM fluxes from the Mississippi, Mobile, and Apalachicola Rivers. In the inner shelf, the color signal becomes even more complicated as the introduction of waters from Suwannee, Hillsborough, Peace, and Caloosahatchee Rivers mix with the above water masses, as well as with those waters created locally from high energy mixing (waves, long-shore currents, etc.) and heat flux imbalances.

The ecological/optical conditions on the WFS are as complicated as any coastal region, yielding situations where the chlorophyll a biomass may range from 0.01 to >20 μg liter^{-1} at the same location during different time periods. When oligotrophic waters dominant the shelf, bottom features are clearly evident in high-resolution hyperspectral data to a depth of 30 meters. At other times, river and estuary waters dominate, and the bottom is undistinguishable in waters <2 meters deep. In between these two conditions, the color signal is mainly a function of the ecological interactions between phytoplankton growth and loss and CDOM creation and destruction. Within the inner shelf, the color signal is further modified by the bottom classification and sediment re-suspension. Our goal on the WFS is to derive and validate a set of fundamental ecological/optical/physical equations that addresses, and eventually predicts, the complexity of the IOPs and the resultant water-leaving radiance. This site is an ideal location for the regional time and space scales being studied.

WORK COMPLETED - 2002

The work in FY2002 continued the integration of the radiative transfer code with the simulated IOPs from the EcoSim 2.0 (ES2) 2-dimensional WFS solutions. The previous work demonstrated the ability to use simulated IOPs to generate $Rrs(\lambda)$ spectra, however, computation speed and radiometric accuracy was an issue. In conjunction with Dr. C. Mobley (N0001497C0019 and N00014D01610002), we have integrated a very fast, radiometrically robust, radiative transfer code (Ecolight 4.1) with the ES2 IOP output IOP data stream. This code is now to be integrated into a 3-dimensional IOP simulation, and this work should be completed by Spring 2003.

In addition to the numerical coding challenges faced this year, the importance of the estuarine boundary condition became critically evident for predicting the cross-shelf IOP distribution (see also N00014-00-1-0411). The estuarine boundary condition includes not only the CDOM inputs, but also the nutrient and particulate loads to the near-shore environment. It was found that these nutrient inputs were critical in the prediction of particulate absorption and scattering, thus an accurate assessment of inputs was required. This assessment was used to establish the shore-ward boundary condition during periods of peak flows in the Fall of 1998. These fresh water and estuarine data sets are particularly sparse, and their collection required coordination with 8 different state and federal agencies. Frequently the data were inconsistent and required multiple cross-checks and repeat communication with the various agencies. However, all the water quality data from 1997 to 2002 from the Charlotte Harbor region has been assembled in an ArcView database and is available for distribution. This data set forms the basis for the shore-ward boundary condition in the ES2 2-dimensional simulation, as well as for the 3-dimensional runs to be generated in FY2003.

RESULTS -2002

The terrestrial nutrient source hypothesis, which suggests that the intensification of biomass and IOPs in the near-shore environment on the WFS, has often been questioned because fresh water systems appear to be nitrogen limited on the West Florida Shelf. This appearance is the result of decades of measurements of the Dissolved Inorganic Nitrogen (DIN) to Dissolved Inorganic Phosphate (DIP) ratio of some terrestrial source waters, which are frequently below that which is considered necessary for balanced phytoplankton growth (mol DIN:mol DIP = 16:1). This has been particularly true for studies in the Charlotte Harbor region because the Peace River, which supplies >70 percent of the fresh water to the upper harbor estuary, frequently has DIN:DIP ratios <0.1. The cause of this extremely low value is that the Peace River drains the Hawthorne phosphatic formations, and frequently has DIP concentration that are an order of magnitude greater than the other rivers that supply fresh water to Charlotte Harbor. However, this apparent excess in phosphorus disappears if Total Nitrogen (TN), which also includes Dissolved Organic Nitrogen (DON) and Particulate Organic Nitrogen (PON), is considered as well as DIN. TN values can be orders of magnitude greater than DIN and may provide a source of nitrogen to the ecological system that directly, or indirectly, may be used by the phytoplankton community. Support for this supposition can be found in the high levels of ^{14}C productivity measurements in the Harbor when DIN is undetectable. TN to Total Phosphorus (TP) in the Peace River has been estimated to be ~16.

The Charlotte Harbor region can be divided into upper and lower estuaries (Figure 1). The fresh water of the upper estuaries is mainly supplied by the Peace and Myakka; the lower estuary is supplied by the Caloosahatchee River. The upper estuary is flushed mainly through Boca Grande Pass and around

Pine Island, while the lower estuary is flushed mainly through San Carlos Bay. The lower estuary is much smaller in size and half as deep as the remainder of the Charlotte Harbor region, and as a result has an order of magnitude smaller volume associated with it (1.0×10^8 m^3 versus 1.3×10^9 m^3). Fresh water flows are greater through the Caloosahatchee River than the Peace River as it drains both the Caloosahatchee River basin and Lake Okeechobee. The larger flows and smaller volume yield much smaller residence times for the fresh flow into the lower estuary compared to the upper estuary. In addition, the Caloosahatchee basin and Lake Okeechobee are not as impacted by the Hawthorne formations, and as a result the Caloosahatchee River has an order of magnitude smaller TP concentration than the Peace River, yielding a TN:TP ratio >25.
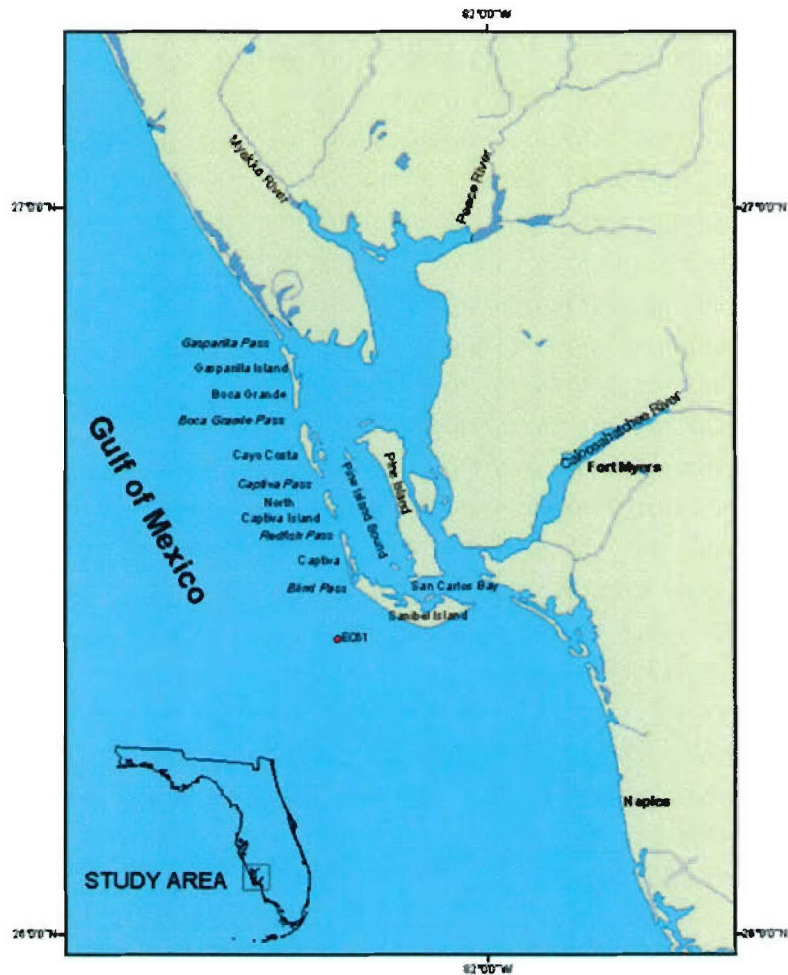

Figure 1. Study area in and around the Charlotte Harbor Estuary.

Flows from the Peace and Caloosahatchee River are frequently of similar size, however the shorter residence time of the Caloosahatchee estuary (lower Charlotte Harbor) both complicates and simplifies the calculation of total nutrient delivery to the shelf. The complications arise from the fact that modification of the nutrient during high water flow pulses during their transit through the lower will be far less than those in the upper harbor. In 2001, the water flows were sufficient to completely turn the entire lower estuary over twice in one week. Thus, one could assume very little modification of the particulate carbon, nitrogen, and phosphorus. However, with the longer residence times of the upper harbor, a large fraction of the water is delivered to the shelf with some indeterminate nutrient history.

We have attempted to correct for these effects by collecting a large series of data from the rivers, middle harbor, and near-shore environments and regressing the inorganic and organic nutrients against salinity (Figure 2). While the some spread in the data, it appears that the modification through the estuary of the total nutrient stocks is low and that a linear extrapolation is sufficient. Evidence for optical impacts of these high water pulse events can be seen in satellite, mooring, and ship data.
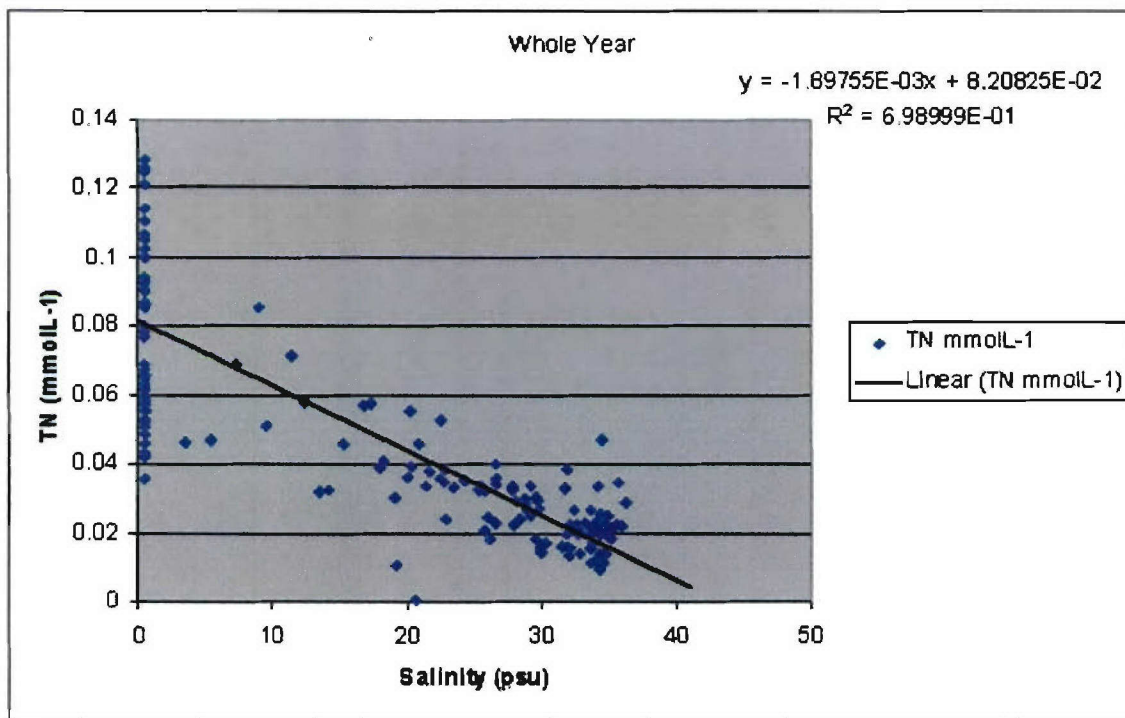

Figure 2. Total Nitrogen during 1998 and 1999 from West Florida Shelf/Charlotte Harbor region.

The biomass results of adding these nutrient pulses can be seen in Figure 3, where the total chlorophyll concentrations are greatly increased in the near-shore areas. This is matched by increase in chlorophyll seen in the SeaWiFS estimated chlorophyll (Figure 4 and 5).
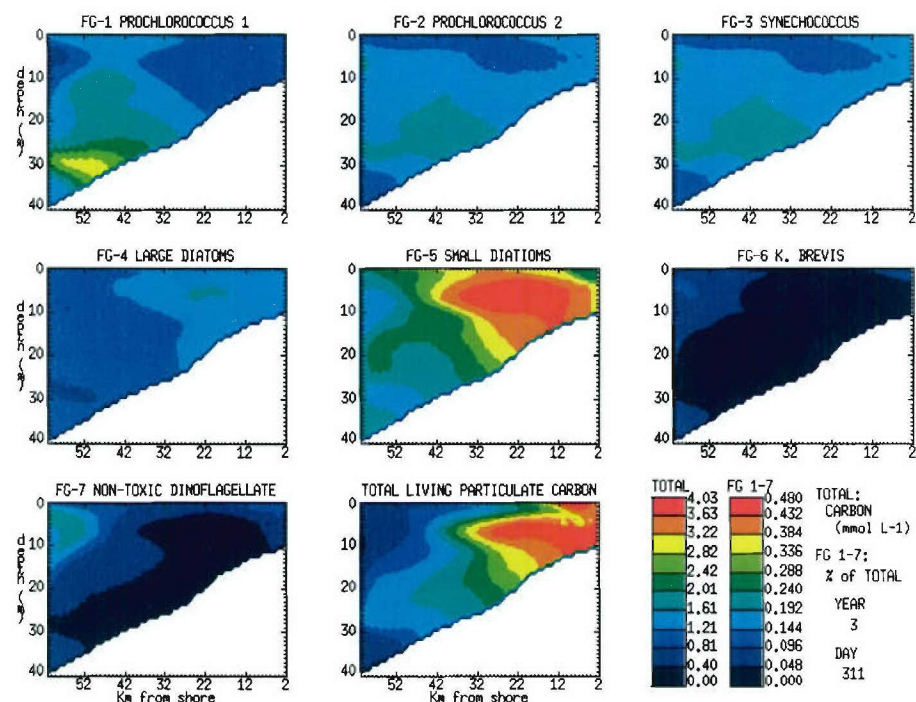
Figure 3. Predicted chlorophyll and functional group distribution for day-of-year 311 (November 7th).
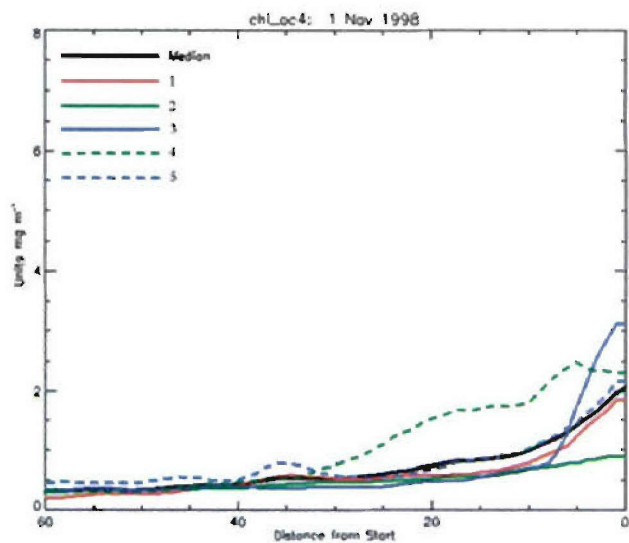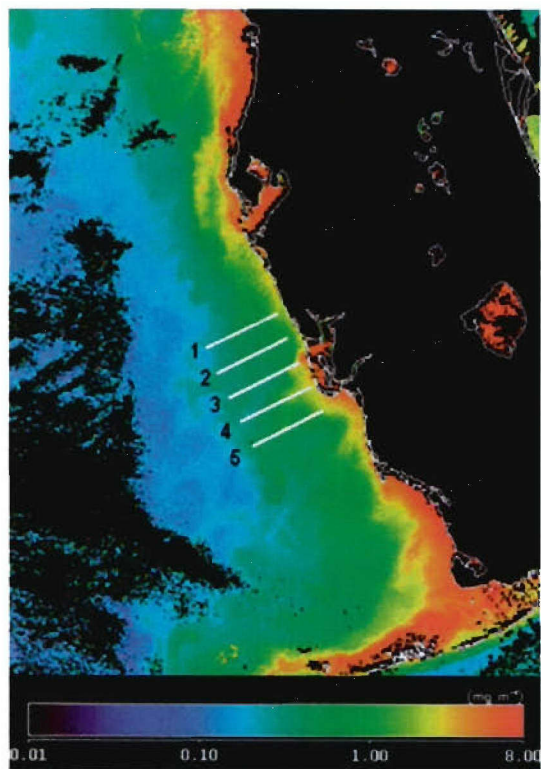
Figure 4. SeaWiFS estimated chlorophyll a concentration for the West Florida Shelf and selected transects on November 1, 1998.
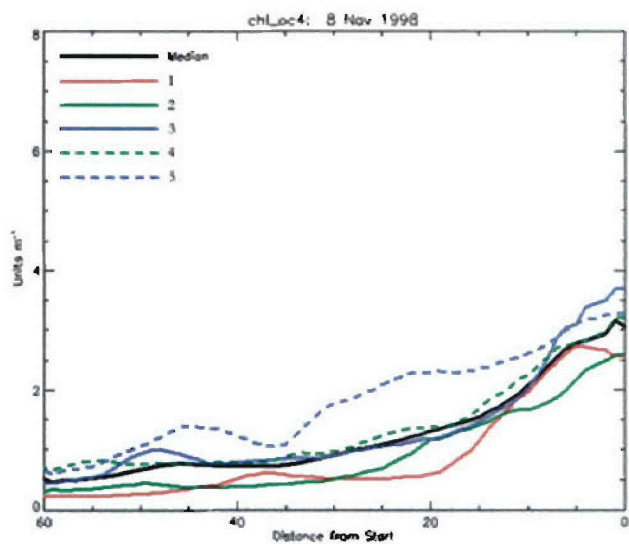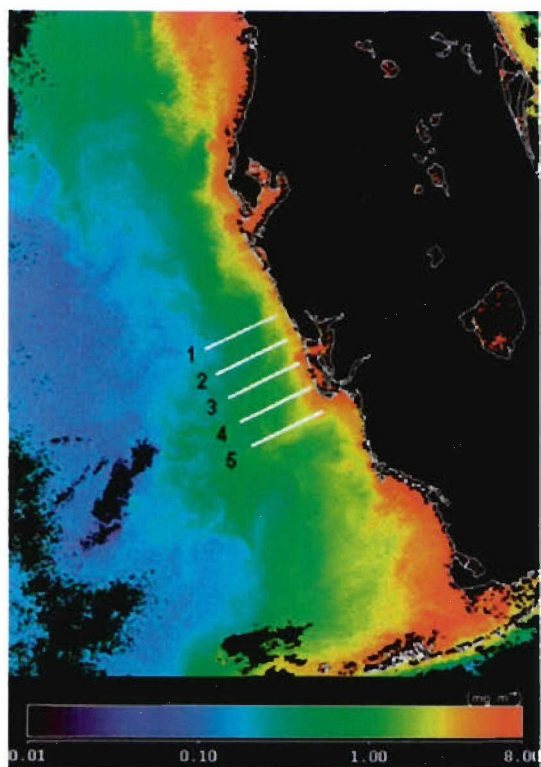
However, the predicted $R_{rs}(412)$ and $R_{rs}(443)$ values are not as satisfying to review (Figures 6 and 7). While it appears that we may have achieved an adequate representation of the increase in biomass (and CDOM, see N00014-00-1-0411), the remote sensing reflectance values are obviously much lower and appear to change off-shore/on-shore relationship between November 1st and November 8th. The lower values can sometimes be attributed differences in illumination inputs to the radiative transfer calculations. However, the change in the off-shore/on-shore gradient on November 8th suggests that something fundamental may be different between our simulated IOPs and the resultant R_{rs} values, versus those estimated from SeaWiFS. One can speculate that since a tropical storm just passed through the region, a tremendous amount of sediments may have been re-suspended, adding a significant backscattering component that was not incorporated into the ES2 simulation. This would appear plausible since both the OC4 Chlorophyll a algorithm (Figure 5) and the Carder $a_{dg}(412)$ (Figure 2 of N00014-00-1-0411) algorithm both suggested increases in the near-shore following the storm, even while the absolute magnitude of the spectral R_{rs} values are increasing. It does appear that this scattering effect has dissipated by December 4th (Figure 8, 9, and 10) and a better correlation between the off-shore/on-shore gradient in predicted and measured R_{rs} is found. However, the magnitude of the predicted R_{rs} values is still much too low, suggesting a problem with the scattering sections of combined ES2/Ecolight system. A further exploration of these results is anticipated in FY2003.

Figure 6. SeaWiFS estimated and ES2 predicted $R_{rs}(412)$ and $R_{rs}(443)$ for the West Florida Shelf and selected transects (see Figure 4) on November 1, 1998.
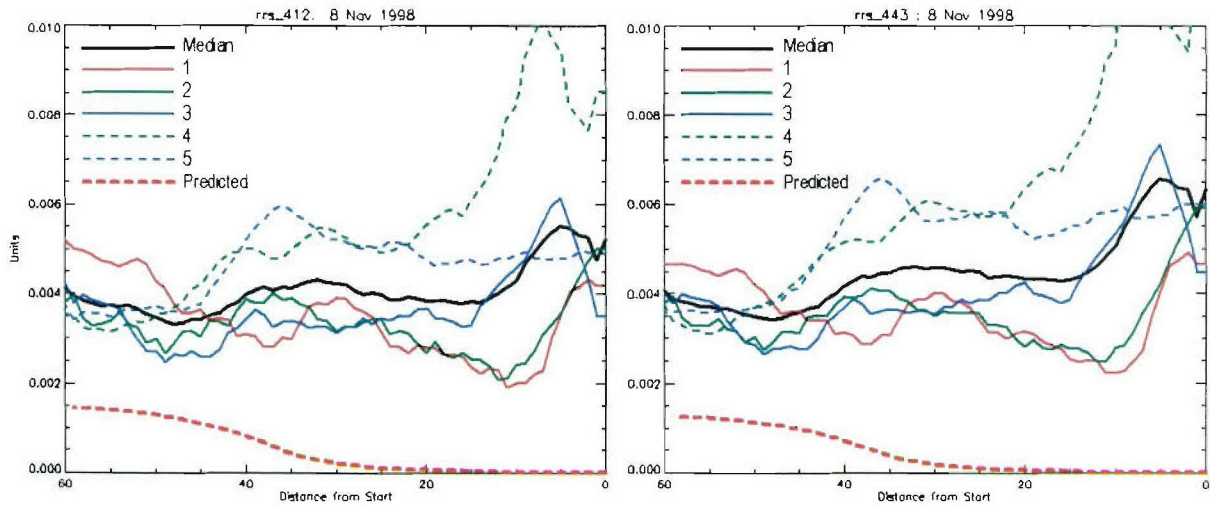
Figure 7. SeaWiFS estimated and ES2 predicted $R_{rs}(412)$ and $R_{rs}(443)$ for the West Florida Shelf and selected transects (see Figure 4) on November 8, 1998.
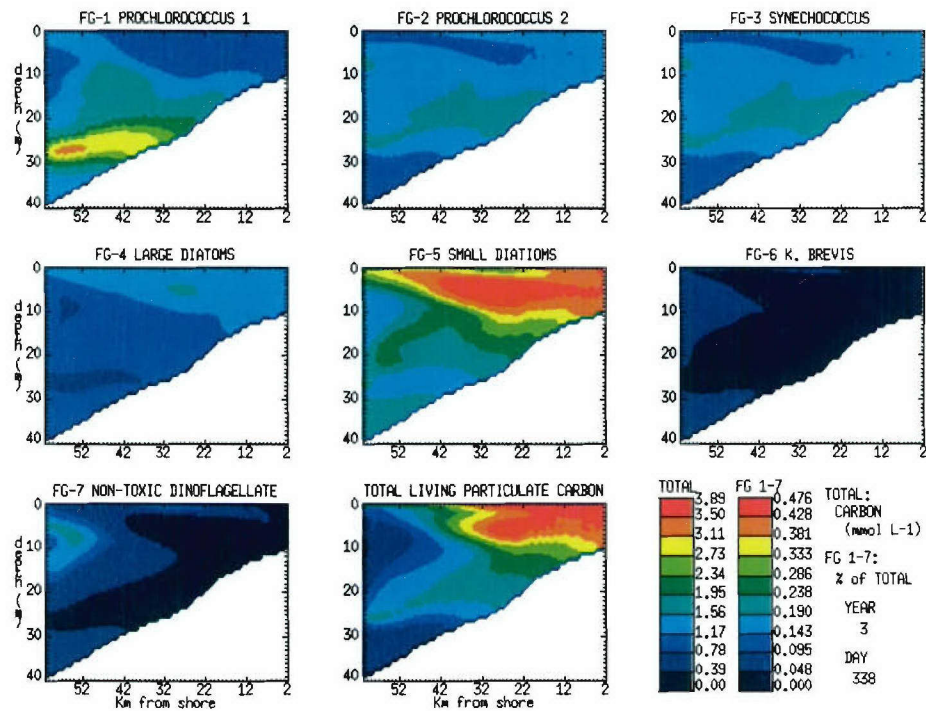
Figure 8. Predicted chlorophyll and functional group distribution for day-of-year 335 (December 5th).
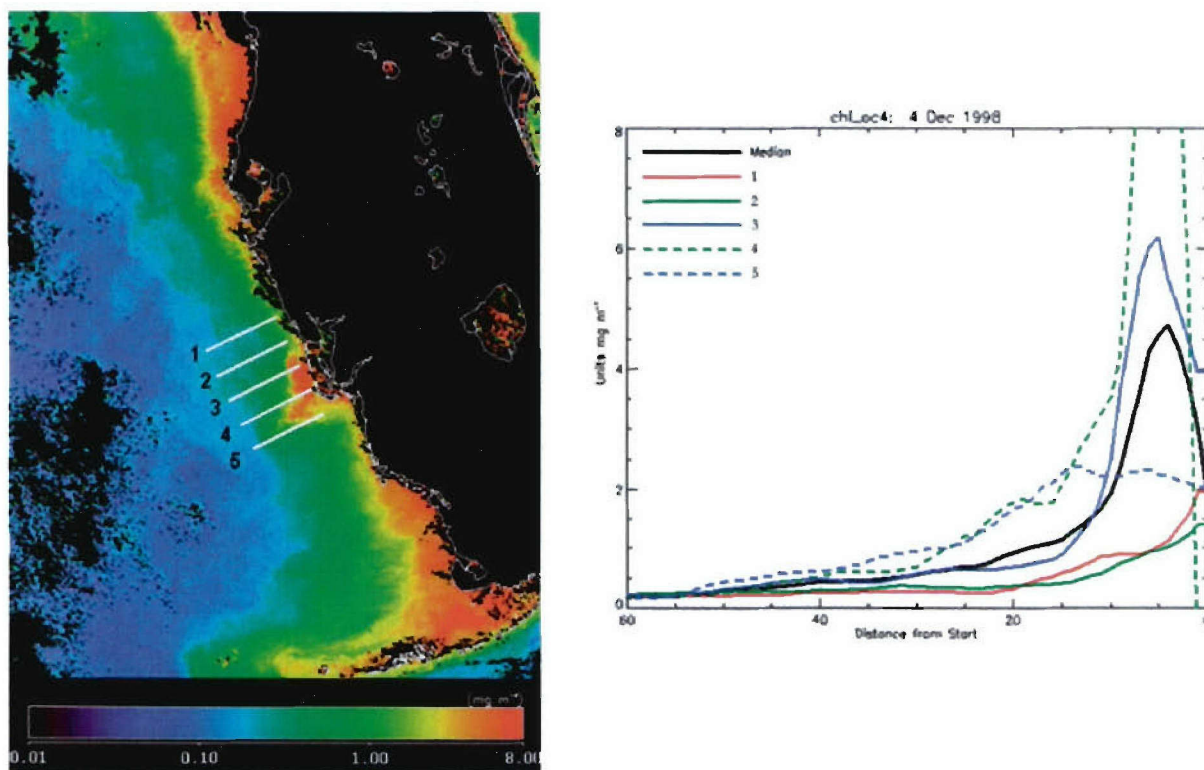
Figure 9. SeaWiFS estimated chlorophyll a concentration for the West Florida Shelf and selected transects on December 4, 1998.
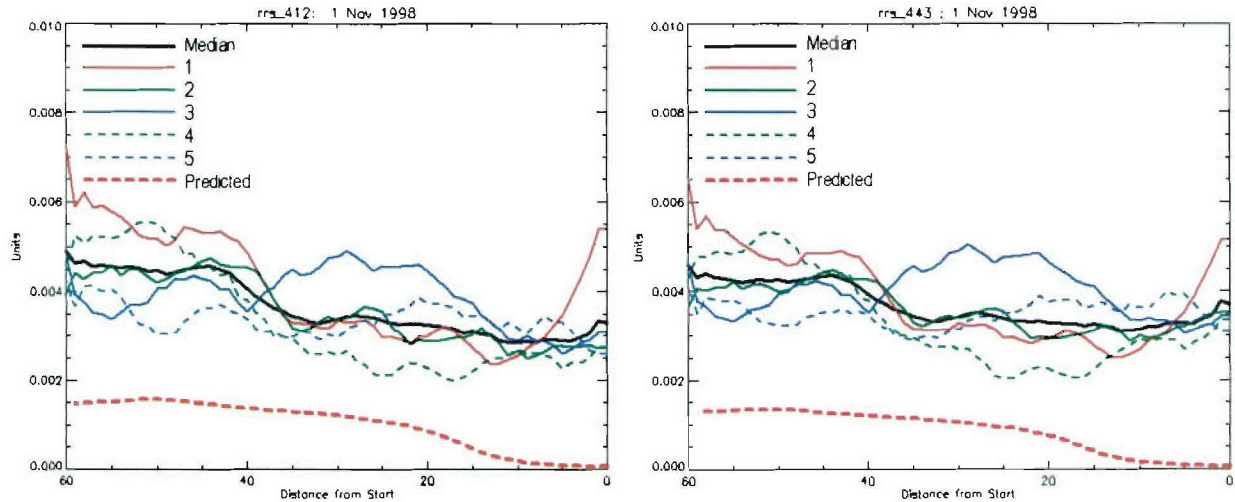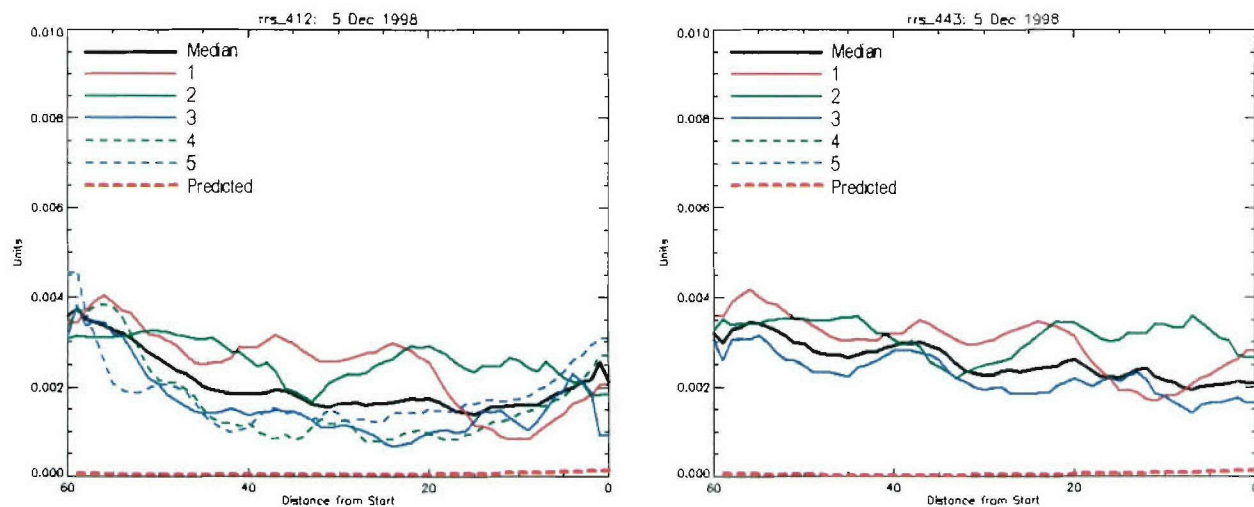

Figure 10. SeaWiFS estimated and ES2 predicted $R_{rs}(412)$ and $R_{rs}(443)$ for the West Florida Shelf and selected transects (see Figure 4) on December 4, 1998.

WORK COMPLETED -2003

The work in FY2003 focused on publication of ecological and optical results from the 2-D simulation of the WFS. With the integration of the shoreward boundary condition for nutrients and color, the simulation showed robust comparisons to the satellite imagery for 1998 (see also Progress Report

Bissett, N000140010411, for a discussion on the CDOM impacts of the shoreward boundary condition). In addition, the use of HPLC data, collected during November 1998, allowed us to validate the ecological predictions of phytoplankton competition with respect to differential light and nutrient utilization. These results have been submitted for publication in a volume of UNESCO Monographs on Oceanographic Methodology-Manual on Harmful Marine Microalgae (Bissett et al., 2005).

In conjunction with Dr. C. Mobley (N0001497C0019 and N00014D01610002), we have integrated a very fast, radiometrically robust, radiative transfer code (Ecolight 4.1) with the ES2 IOP output data stream. This integrated EcoSim/Ecolight formulation allows us to directly simulate remote sensing reflectance, $Rrs(\lambda)$, which may be compared directly to satellite and aircraft remote sensing data. This allowed us to explore errors in the simulated IOP fields, as well as focus on the possible errors in the satellite derived IOP field in near-shore waters. In addition, the downwelling irradiance model used in EcoSim to drive the time-dependent ecological change in IOPs is an approximation, which was derived in an earlier version of EcoSim (Bissett et al., 1999; Bissett et al., 1999). The results of these approximations were tested against the more robust radiative transfer model, Ecolight, and the results of the error analysis between these models are being prepared to be submitted for publication.

Lastly, our plan to generate a 3-dimensional prediction of upwelling radiance on the West Florida Shelf was based on a circulation model developed by the University of South Florida. However, this POM based code is not sufficiently robust to be used in this manner. We have decided instead to focus on the ROMS/TOMS code development (see Progress Report Schofield, N000149910196, and Bissett, N000149910198). In addition to being developed under an open source agreement between multiple institutions, it is being designed to have nested grids for multiple spatial scale resolutions, as well as being transportable to many different massively parallel computer platforms. We believe that this is the best approach to generate a code set that is more likely to be transitioned to the naval, geophysical, and biogeochemical research community.

RESULTS - 2003

The ecological results demonstrate the importance of the terrestrial influences on the IOP distributions. In particular, the increase in nutrient concentrations driven by terrestrial fluxes from the Charlotte Harbor Estuary show orders of magnitude increase in nitrogen, silica, and phosphorus in both organic and inorganic forms (Bissett et al., 2005). These nutrient fluxes led to phytoplankton accumulations that were both remotely sensed by SeaWiFS and simulated in this study. Figure 11 shows the satellite estimated and simulated surface total chlorophyll following Hurricane Georges and Tropical Storm Mitch. The simulated nearshore values without the pulse of estuarine water from Charlotte Harbor are clearly outside of 1 standard deviation (s.d.) of the satellite estimated chlorophyll a concentration. The very high simulated values nearshore on November 8th appear to result from the inability of the 2-D physical simulation to adequately resolve the 3-D baroclinic flows around the southern end of the simulation range.

a Total Chlorophyll 1 Nov 1998

Legend:
- Mean +/- 1 Standard Deviation
- Mean of Lines 1-30
- Charlotte Harbor Lines 22-30
- EcoSim Top 5m (pulse-Case2)
- EcoSim Surface (pulse-Case2)
- EcoSim Top 5m (no pulse-Case1)
- EcoSim Surface (no pulse-Case1)

y-axis: mg chl (m^{-3})
x-axis: Distance from 10m isobath

b Total Chlorophyll 8 Nov 1998

Legend:
- Mean +/- 1 Standard Deviation
- Mean of Lines 1-30
- Charlotte Harbor Lines 22-30
- EcoSim Top 5m (pulse-Case2)
- EcoSim Surface (pulse-Case2)
- EcoSim Top 5m (no pulse-Case1)
- EcoSim Surface (no pulse-Case1)

y-axis: mg chl (m^{-3})
x-axis: Distance from 10m isobath

Figure 11: Simulated versus SeaWiFS Total Chlorophyll. (a) November 1, 1998, and (b) November 8, 1998. The simulated chlorophyll a values are within 1 standard deviation (s.d.) of the average satellite estimates across the shelf in the simulation runs which include a shoreward boundary condition (solid red and green lines). Without the shoreward boundary conditions, the nearshore simulated values drop below 1 s.d. of the satellite estimates. The higher values nearshore on November 8th overestimate the mean conditions, but are similar to the Charlotte Harbor estimates. (Figure 12 shows the model domain)

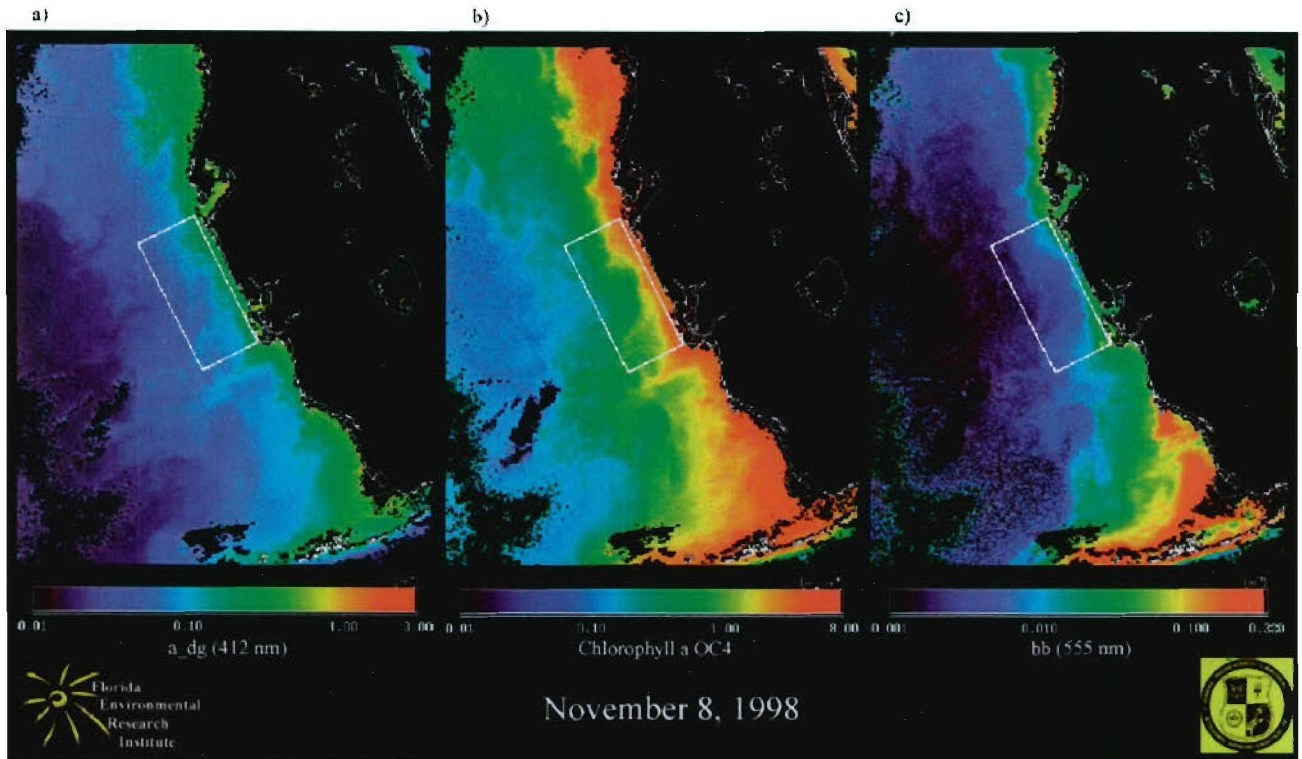*Figure 12: The West Florida Shelf, November 8, 1998. SeaWiFS estimated (a) absorption at 412m, $a_{dg}(412)$; (b) chlorophyll a (OC4 algorithm), and (c) backscattering at 555 nm, $b_b(555)$. The model domain is shown as the white box on each of the images. The SeaWiFS line plots on Figure 11 are derived by dividing the domain into 30 equally spaced lines and averaging them to create a statistically significant data set to compare against the 2-D simulation results. (a), (b) and (c) show the influence from local terrestrial freshwater sources of nutrients on the total color and chlorophyll signal in the model domain. Evident in the color and chlorophyll signals are the high concentration just south of the model domain and Charlotte Harbor, which was not adequately resolved by the 2-D physical circulation model. This is the source of some of the errors in 11.*

While the estimates of total chlorophyll and the distributions of chlorophyll amongst phytoplankton functional groups are reasonable in light model deficiencies (Bissett et al., 2005), the simulated backscattering errors appear to be more systematically lower than the satellite estimates (Figure 13). These errors appear to result from 1) an inaccurate description of phytoplankton backscattering, 2) exclusion of sediments in the simulated IOPs, and 3) possible inaccuracies in the estimate of backscattering from the satellite signal. The first two sources of error are clearly problems that need to be addressed. The backscattering in EcoSim is currently a function of the total chlorophyll a concentration, developed for Case 1, open ocean conditions (Morel and Maritorena, 2001). While this formulation appears to be reasonable in the offshore region, it becomes more problematic nearshore. Figure 13b contains the satellite and simulation results following TS Mitch, and the nearshore backscatter is tremendously higher than Figure 13a (note the scale shift). The passage of a tropical storm would probably resuspend a fair amount of bottom sediments in this shallow water region, and it is highly likely that the exclusion of this IOP component is the reason for part of the error.

a Backscatter 1 Nov 1998

Mean +/- 1 Standard Deviation
Mean of Lines 1-30
Charlotte Harbor Lines 22-30
EcoSim Top 5m (pulse-Case2)
EcoSim Surface (pulse-Case2)
EcoSim Top 5m (no pulse-Case1)
EcoSim Surface (no pulse-Case1)

b Backscatter 8 Nov 1998

Mean +/- 1 Standard Deviation
Mean of Lines 1-30
Charlotte Harbor Lines 22-30
EcoSim Top 5m (pulse-Case2)
EcoSim Surface (pulse-Case2)
EcoSim Top 5m (no pulse-Case1)
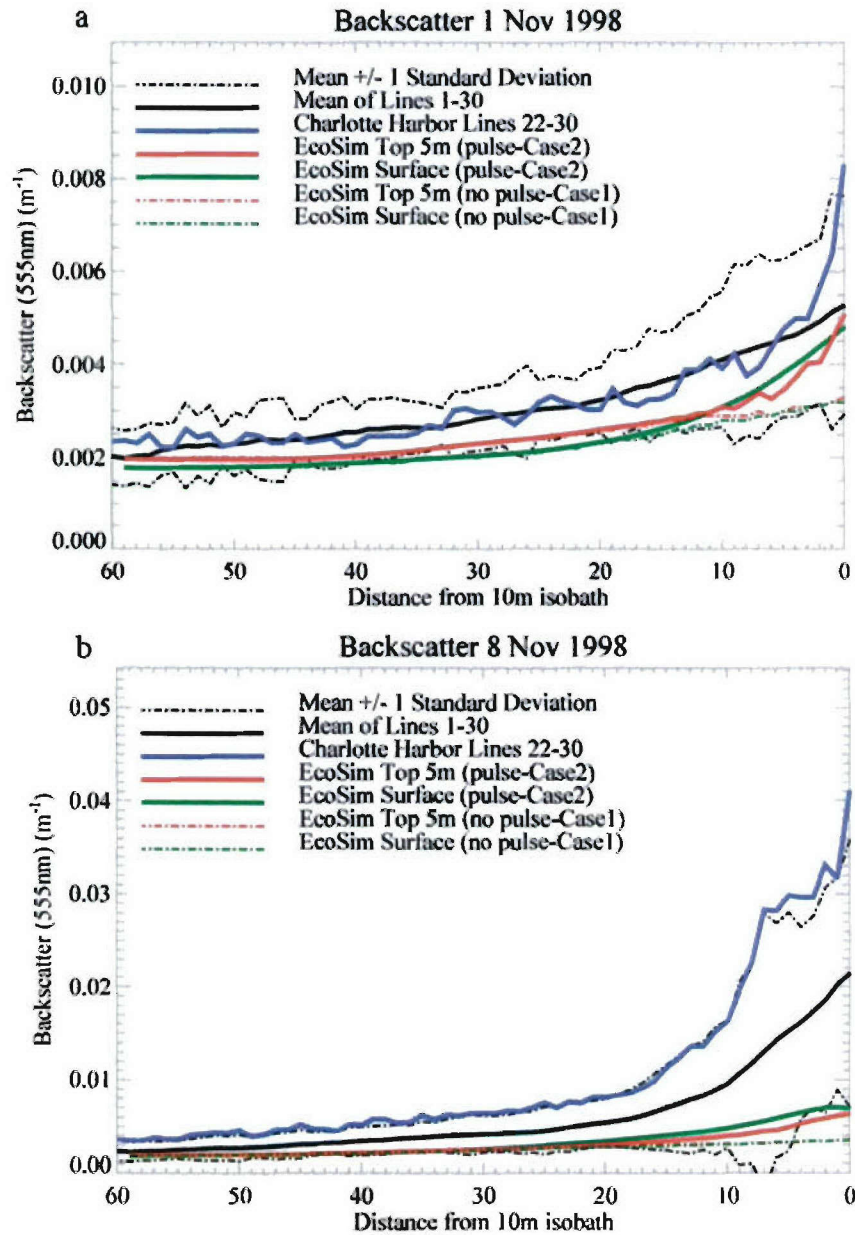EcoSim Surface (no pulse-Case1)

Figure 13: Simulated versus SeaWiFS Backscattering at 555 nm. (a) November 1, 1998, and (b) November 8, 1998. The simulate values are within 1 standard deviation (s.d.) of the average satellite estimates across the shelf in the simulation runs which include a shoreward boundary condition (solid red and green lines). Without the shoreward boundary conditions, the nearshore simulated values drop below 1 s.d. of the satellite estimates. The simulated values are systematically lower than the satellite estimates, possibly the results of 1) poor model formulation, 2) exclusion of sediment IOPs, 3) errors in the satellite formulation.

However, there was also a dramatic shift across the entire region in the satellite $R_{rs}(555)$ estimates (Figure 14) from November 1st to November 8th (again note the scale shift). It is unclear why there would be such a dramatic change, and this shift is currently under study. In addition, the errors between the satellite R_{rs} and the simulated R_{rs} across all wavelengths are much greater than the IOP products themselves. This too needs to be resolved. The satellite R_{rs} products are taken from the APS

processing of the SeaWiFS data (R. Arnone, NRLSSC) and are derived differently than NASA's SeaWiFS processing in coastal waters to remove bottom and atmospheric contamination effects. This comparison of predicted versus satellite and aircraft R_{rs} will be one of the focuses in FY 2004. These ecological and optical results are more fully described in submitted publications (Bissett et al., 2005; Bissett et al., 2005).
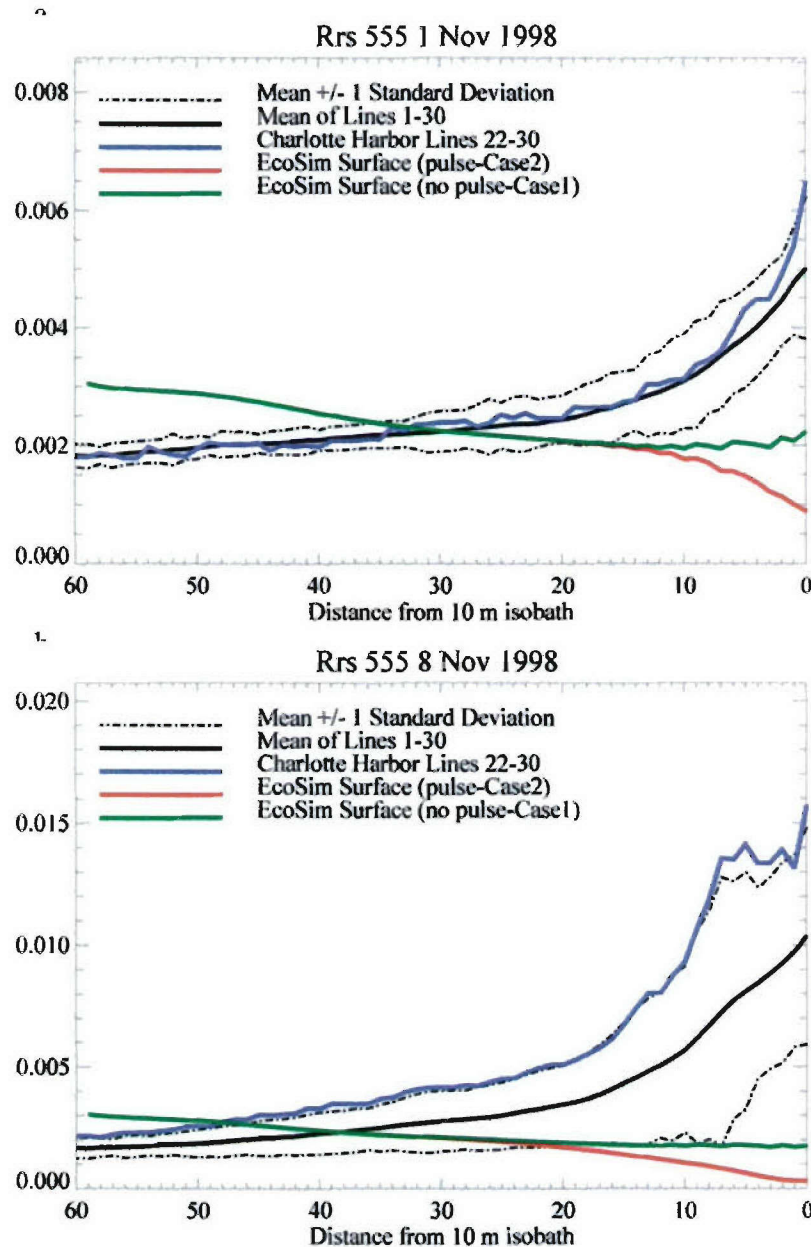

Figure 14: Simulated versus SeaWiFS Remote Sensing Reflectance at 555 nm. (a) November 1, 1998, and (b) November 8, 1998. These errors require addition study to understand. There is a clear scale shift following TS Mitch. In addition, the pattern of errors is not similar to the IOP errors for Figures 11 and 13. The resolution of these errors will require re-evaluating the NRLSSC Rrs calculations as well as the EcoSim/Ecolight coupling.

Lastly, initial comparisons of the EcoSim downwelling approximations versus the more robust Ecolight downwelling calculations, using the same simulated IOP distributions, has yielded some interesting results (Figure 15). The errors between the propagation of downwelling irradiance appear most evident at lower light levels, and at high b/c values (data not shown). The EcoSim and Ecolight AOP solutions will also be further explore in FY 2004.
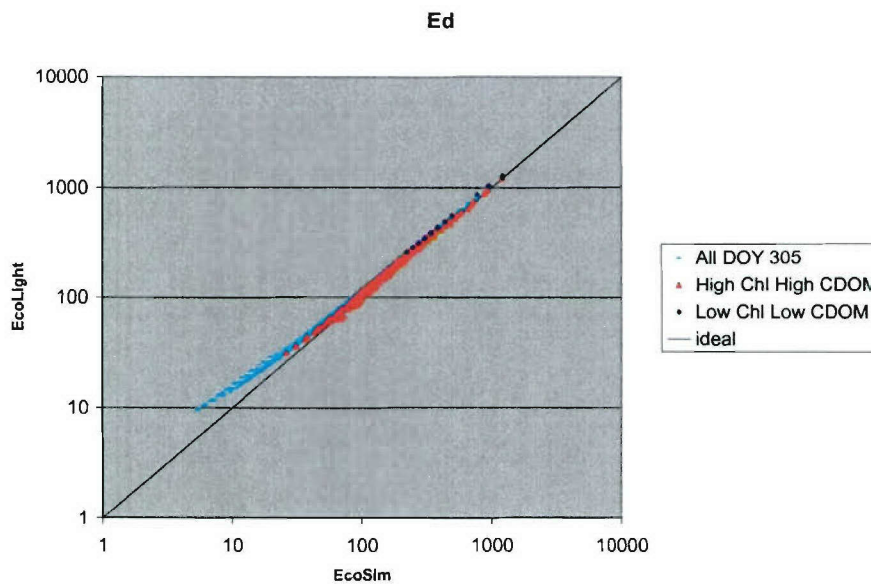

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Figure 15: Ecolight versus EcoSim Downwelling Irradiance Comparison (data in μmol quanta m^{-2} s^{-1}). These were calculated over all depths and all horizontal grid point in the EcoSim 2-D model domain. The data shows very good agreement (nearly 1:1) except at light levels below ~80 μmol quanta m^{-2} s^{-1}.

WORK COMPLETED - 2004

As mentioned in the preceding year's progress report, the previously developed Princeton Ocean Modeling developed for the WFS was not optimized for high performance computing. In addition, it did not contain the terrestrial boundary conditions that were deemed necessary to accurately resolve the near-shore IOP distribution (Bissett et al., 2005). Thus, we sought to build upon the Regional Ocean Modeling System (ROMS; http://marine.rutgers.edu/po/index.html), and its ONR funded follow-on, Terrain-following Ocean Modeling System (TOMS; http://www.ocean-modeling.org/).

What became clearly evident on the WFS was that the physical modeling was of paramount important to the prediction of the IOPs. The IOPs are directly related to the mass constituents in the water column, e.g. absorption and scattering are in a large part a function of the pigmented algal biomass. The mass constituents have time-dependent change characteristics that are approximated in time/space as advection, diffusion, sources, and sinks equations. Thus, the 0-order problem for the prediction of IOPs is the initialization and boundary conditions of all the mass and momentum in the model. The 1-order problem is then the advection and diffusion of the masses; and the 2-order problem is the time-dependent sources and sinks. The order of importance of these problems is dependent on the time

horizon of the forecast (today versus next year). If one is attempting to develop predictive simulations over the short-term, operational time horizon, then initialization, boundary conditions, as well as advection and diffusion become critical to the production of a successful forecast.

This has led us to partner with the physical modeling group at Rutgers University (RU), who are in a large part leading the development of the ROMS/TOMS code. In addition, the RU Coastal Ocean Observation Laboratory (COOL; http://marine.rutgers.edu/cool/) is in the midst of a 5 year NSF Coastal Ocean Process grant (Lagrangian Transport and Transformation Experiment, LaTTE; http://marine.rutgers.edu/cool/latte/index.htm) to discern the impacts of the Hudson River on the biogeochemical dynamics of the Mid-Atlantic Bight. A major component of this program is a dye injection program, which seeks to serve as initialization and validation data for a 4-D physical data assimilation modeling program. This program offered the abilities to couple the ecological modeling with a high resolution physical modeling effort that was focused on the buoyancy driven impacts on coastal ocean circulation. At the same time, the biogeochemical group included past ONR funded optical scientist who could provided the initialization/validation data required for the ecological/optical simulation. These combined efforts surpassed the programmatic operations on the WFS, and for this reason, we sought and obtained permission for ONR to refocus our WFS efforts on the Hudson River area of the Mid-Atlantic Bight.

This process was added by previous work with the ROMS code, version 1.8. However, during the past year the ROMS code under went two revisions, 2.0 and 2.1. These revisions were significant in terms of the differences in memory management and parallelization. As EcoSim is a subroutine in the ROMS code, and is developed off line of the main ROMS effort, it was frequently difficult to coordinate coding efforts. The major effort for year went into recoding EcoSim under a strict MPI regime prescribed by Hernan Arango, Rutgers University. All subroutines, initialization and parameterization files, and I/O routines were made identical to all other ROMS mass tracer routines. H. Arango was critical to this effort, and while the initial coding was difficult, the EcoSim code has now been released as part of the ROMS 2.1 code set.

One advantage to this effort was that the RADTRAN spectral light model (Gregg and Carder, 1990), which was previously run in an offline mode, has now been fully incorporated into the ROMS code. This was important for two reasons. The first is that these light data files were very large, and difficult to hold in the cache space of the individual processors on the massively parallel machines for which this code is optimized. The second benefit is that previous offline RADTRAN runs required the user to specific time and place for each location. If the model domain was large, particularly in the north/south direction, i.e, the entire Mid-Atlantic Bight, then there would be significant differences in the light as a function of latitude. The I/O required to search through these large light files, as well as the difficulty in trying to approximate the longitudinal differences led us to fully incorporate RADTRAN into the ROMS code. This had the added benefit of allowing any ROMS user to run EcoSim anywhere in the world without the need to fully understand spectral optical forcing.

Another advantage to the ROMS/TOMS 2.1 version is that it allows for full nesting of model domains, such that a coastal ROM/EcoSim model could be seamless coupled to a global ROMS/EcoSim model. The means that ecological/optical forecasting may be accomplished by anyone currently running the ROMS code, for any model domain. Additional advantages to the ROMS/TOMS 2.1 modeling effort may be found at http://marine.rutgers.edu/po/index.php.
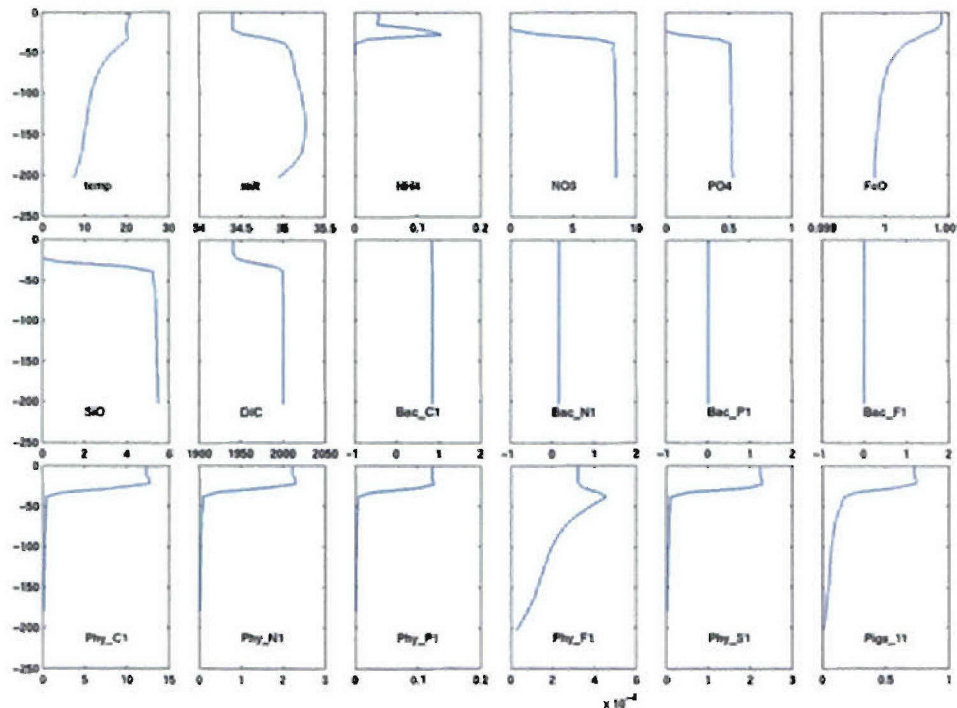

Figure 16. One Dimensional view of ROMS/EcoSim BIOTOY version. This version of the ROMS 2.1 includes a fully integrated 3-D physical model with the EcoSim ecological model in a format that allows the user to quickly test code and parameters. This allows for rapid debugging of the parallelized code prior to running on the DoD HPC computers. It is also a significant education tools that may be used in the transition of EcoSim to a wider user community.

The first step in this latest recoding was to develop a fully 3-D version of the code for an idealized domain that would resemble a 1-D solution. A previous difficulty with the ROMS/EcoSim code development was that the ecological code was developed independently from the physical circulation code. This was done, in part, because of the complexity involved in running the fully parallelized version in order to debug the ROMS/EcoSim code. This created enormous difficulties in coordination of code development. This idealized test case (called BIOTOY), is now incorporated directly into the ROMS development set, allowing any user to select modules of the ROMS code with which to quickly test interactions with EcoSim. The output resembles a 1-D model (Figure 16); however, this output is actually the center point of a 6 x 6 grid that fully utilizes the advection/diffusion modeling capabilities of ROMS. Once this BIOTOY version was completed and tested on Sun Unix workstations, it was then ported to the DoD ERDC Major Shared Resource Center (MSRC) Compaq SC45 (512 CPUs) and tested for parallelization and MPI performance. These tests were successfully completed.

The next step is the creation of the EcoSim initialization and parameterization files for the LaTTE domain. Figure 17 shows the domain and the files for the 0.1 m level of the domain for salinity and CDOM.
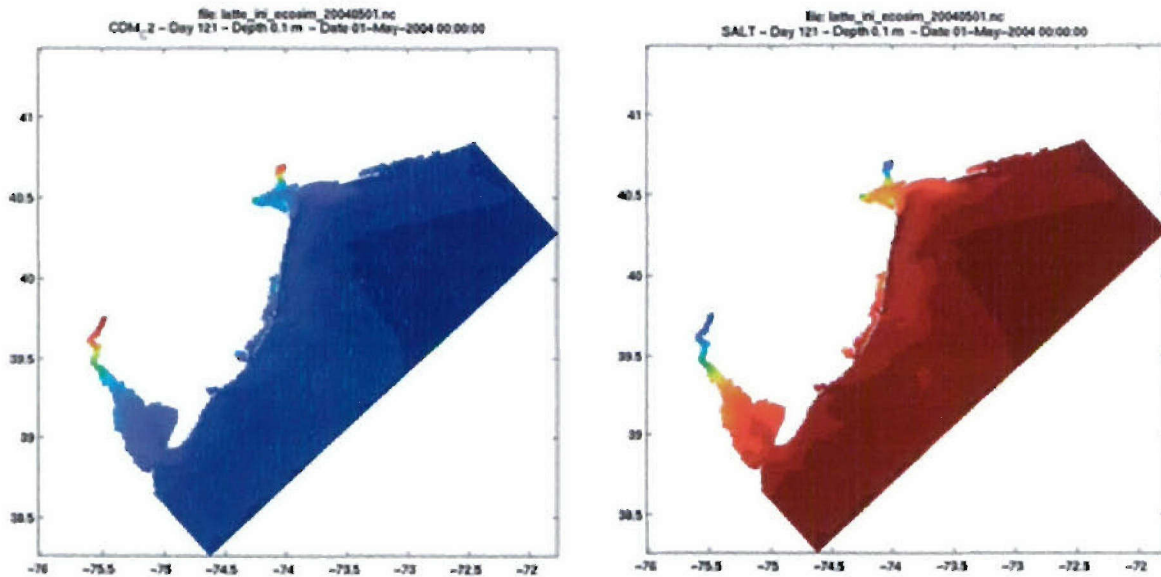

Figure 17. ROMS/EcoSim initialization files for the LaTTE domain. The LaTTE domain includes the Hudson and Delaware River estuaries. The LaTTE project is funded by the NSF Coastal Ocean Processes program, and is focused on the biogeochemistry of terrestrial outflows into the coastal ocean. The project provides a framework by which the physical circulation model is highly resolved and constrained, such that the ecological/optical model may be developed with minimal worries about advection/diffusion errors.

WORK COMPLETED - 2005

Similar to the previous year, ROMS underwent another significant revision to version 2.2. However, this revision included the ability to maintain version control amongst the various ROMS developers. This suggests that the EcoSim code from this point forward with be maintained in each new update to the physical model. Hopefully this will save a lot of recoding of EcoSim with each new version release of ROMS.

In addition to the recoding of the EcoSim module of ROMS, we also ran 3-D simulations testing this code for the LaTTE region during their field campaign during April of 2005. Figure 18 shows the physical modeling results for April 19th, including the projected dye location after injection on April 11th. Of particular note are the differences in the temperature and salinity of the Raritan Bay Estuary and the Hudson River. The impact on the optical properties from these two water boundary conditions may be seen in Figure 19. A sampling of the simulated ecological results may be seen in Figure 20.

The Hudson River water is laden with higher sediment concentrations, where as the Raritan waters contains more blue absorbing, lower scattering materials. The correct establishment of the nutrient,

biological, and optical boundary conditions for these waters is critical to the successful forecasting of the optical properties over these short-term time periods. This year's work has finally created the code set and development environment where we may now focus on the ecological and optical modeling rather than the computer science of code development.
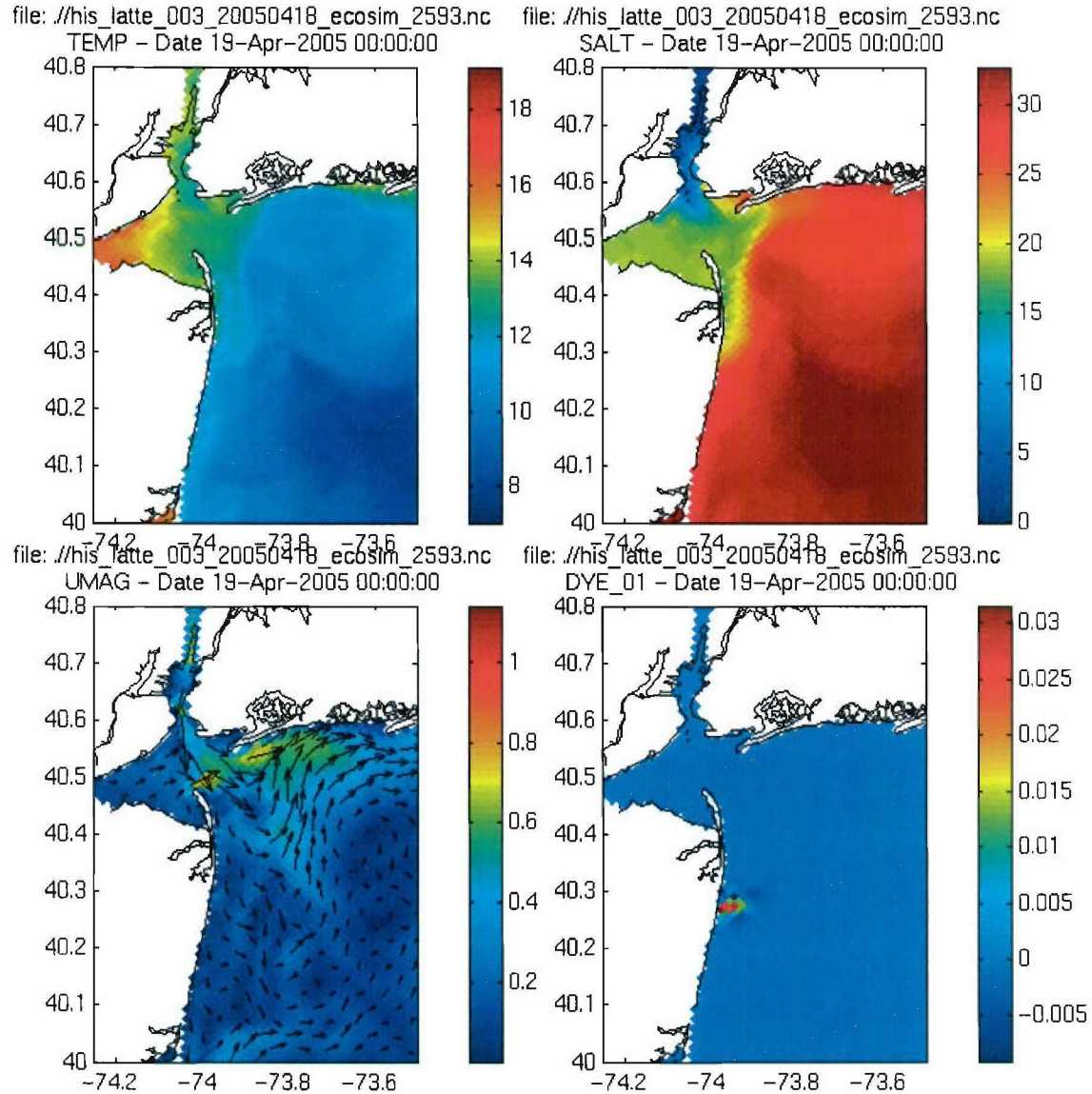

Figure 18. Three-dimensional physical results of ROMS/EcoSim 2.2 version over the LaTTE domain in the Mid-Atlantic Bight on April 19, 2005. Figures in clockwise order from top left hand corner, (1) surface temperature, (2) surface salinity, (3) dye location, and (4) current vectors overlaid on top of U component of the surface current.
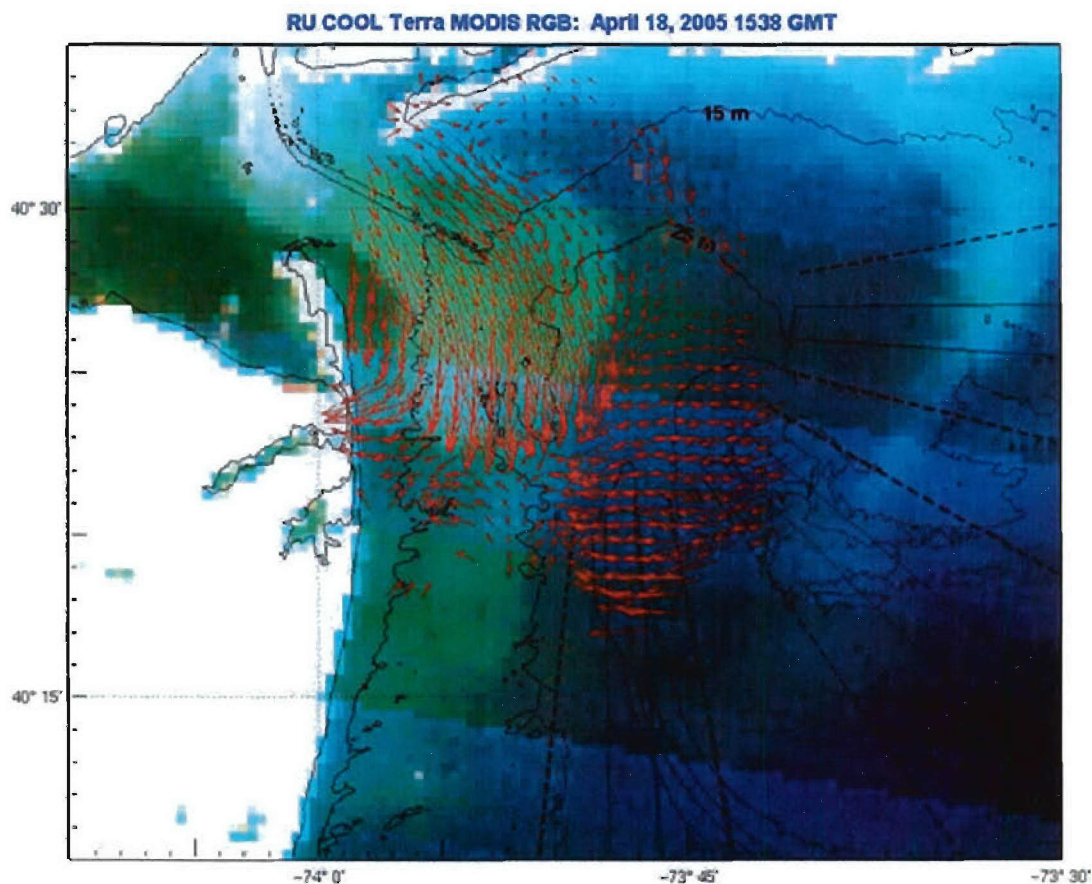
Figure 19. MODIS Terra RGB image of the LaTTE region, with the CODAR surface current field overlaid on the image. The image shows very different optical water masses originating out of the Hudson River and Raritan Bay Estuary (courtesy of Donglai Gong, Rutgers University).

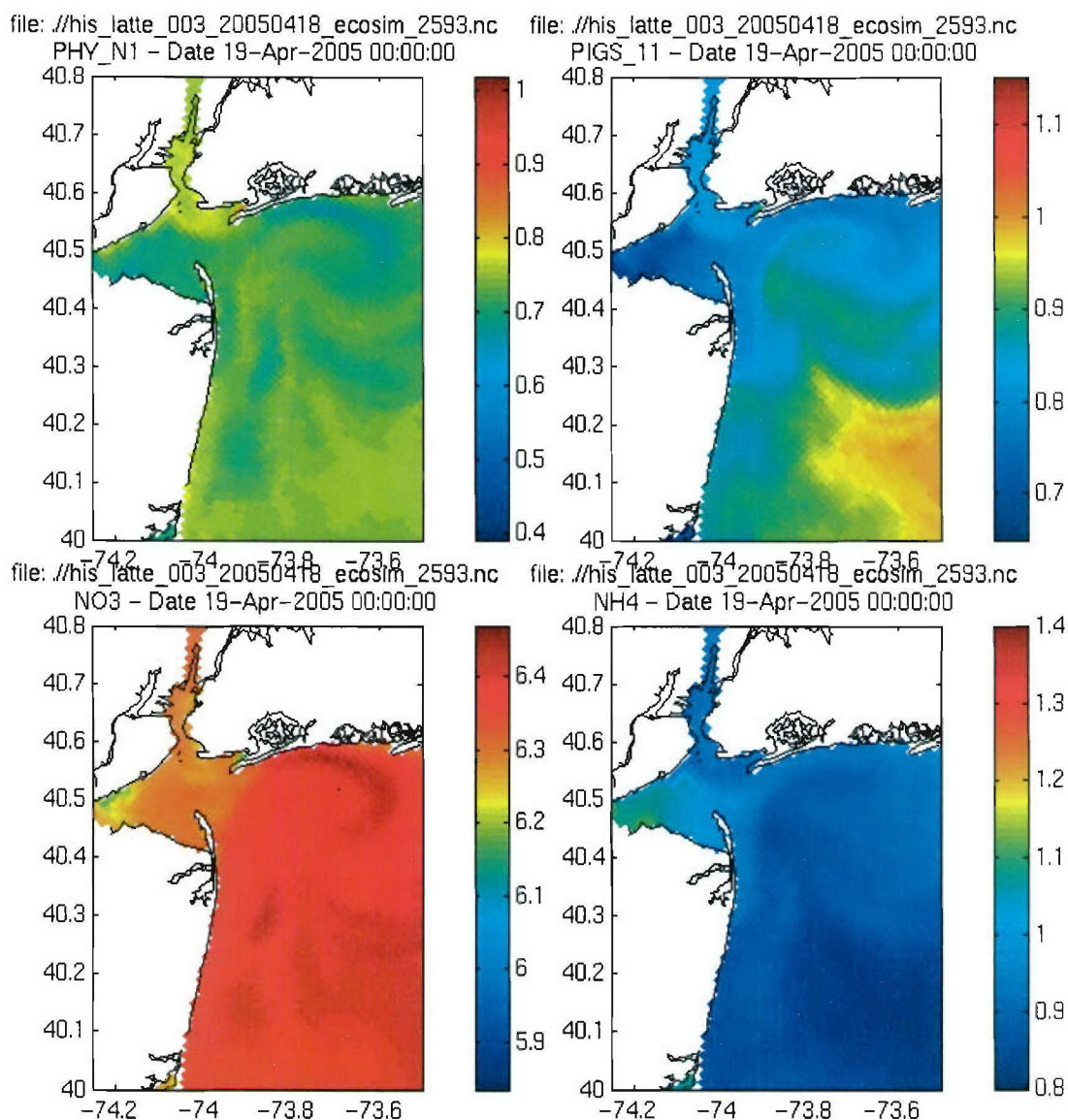(Remainder of this page has been intentionally left blank.)

Figure 20. Three-dimensional ecological results of ROMS/EcoSim 2.2 version over the LaTTE domain in the Mid-Atlantic Bight on April 19, 2005. Figures in clockwise order from top left hand corner, (1) large diatom particulate nitrogen, (2) large diatom chlorophyll a, (3) NH4 concentrations, and (4) NO3 concentrations.

WORK COMPLETED – 2006

This year marked the closing months of this grant. During this period we focused on the integration of Ecolight into a run-time version of the EcoSim code. C. Mobley and L. Sundman decided to pursue this inline coupling of the codes in a PC development environment, outside of the ROMS development loop. This was primarily due to the 1) difficulties we had experienced with coding ROMS subroutines, 2) the ease of code development and results visualization in a PC environment, and 3) their expertise

on this platform. Our role was to help facilitate this code development by providing a compiled version of the EcoSim/ROMS code outside of the C-preprocessor used for UNIX machines, specifically for the BioToy version (6 x 6 grid version). We also provided support for debugging and error checking. We continue to help this effort on other funding.

IMPACT/APPLICATIONS

Forecasting IOPs over operational time horizons of 5 to 10 days will require the ability to directly compare predictions of water-leaving radiance to the data most likely to be used for initialization and validation of the predictions, i.e., aircraft and satellite hyperspectral remote sensing data. This effort will yield a simulation ready to begin direct data assimilation of the water column optical properties to predict absorption and scattering over short-term time horizons.

TRANSITIONS

The EcoSim 2.0 model has been transitioned as part of the open source code of the ONR ROMS/TOMS code set.

RELATED PROJECTS

We are also collaborating with Dr. C. Mobley of Sequoia Scientific, Inc for the coupling of EcoSim with Hydrolight, and Drs. R. Arnone, NRL, and K. Carder, USF, for satellite data analysis.

REFERENCES

Bissett, W.P., Arnone, R., DeBra, S., Dieterle, D., Dye, D., Kirkpatrick, G., Schofield, O. and Vargo, G., 2005. Predicting the optical properties of the West Florida Shelf: resolving the potential impacts of a terrestrial boundary condition on the distribution of colored dissolved and particulate matter. Marine Chemistry, 95: 199-233.

Bissett, W.P., Arnone, R., DeBra, S., Dye, D., Kirkpatrick, G., Mobley, C. and Schofield, O.M., 2005. The Integration Of Ocean Color Remote Sensing With Coastal Nowcast/Forecast Simulations Of Harmful Algal Blooms (HABs). In: M. Babin, J. Cullen and R. Roesler (Editors), MANUAL ON HARMFUL MARINE MICROALGAE. UNESCO MONOGRAPHS ON OCEANOGRAPHIC METHODOLOGY, pp. (in press).

Bissett, W.P., Carder, K.L., Walsh, J.J. and Dieterle, D.A., 1999. Carbon cycling in the upper waters of the Sargasso Sea: II. Numerical simulation of apparent and inherent optical properties. Deep-Sea Research I, 46(2): 271-317.

Bissett, W.P., Walsh, J.J., Dieterle, D.A. and Carder, K.L., 1999. Carbon cycling in the upper waters of the Sargasso Sea: I. Numerical simulation of differential carbon and nitrogen fluxes. Deep-Sea Research I, 46(2): 205-269.

Gregg, W.W. and Carder, K.L., 1990. A simple spectral solar irradiance model for cloudless maritime atmospheres. Limnology and Oceanography, 35(8): 1657-1675.

Morel, A. and Maritorena, S., 2001. Bio-Optical properties of oceanic waters: A reapprasial. Journal of Geophysical Research, 106(C4): 7163-7180.

PUBLICATIONS

Bissett, W. P., Arnone, R., DeBra, S., Dye, D., Kirkpatrick, G., Mobley, C., and Schofield, O.M. (2005). The Integration Of Ocean Color Remote Sensing With Coastal Nowcast/Forecast Simulations Of Harmful Algal Blooms (HABs). UNESCO Monographs on Oceanographic Methodology- Manual on Harmful Marine Microalgae, UNESCO [submitted, refereed].

Mobley, C. D., L. K. Sundman, C. O. Davis, T. V. Downes, R. A. Leathers, M. J. Montes, J. H. Bowles, W. P. Bissett, D. D. R. Kohler, R. P. Reid, E. M. Louchard, and A. Gleason, 2005. Interpretation of hyperspectral remote-sensing imagery via spectrum matching and look-up tables. *Applied Optics* **44**(17), 3576-3592. [published, refereed]

Schofield, O., Bosch, J., Glenn, S., Kirkpatrick, G., Kerfoot, J., Moline, M., Oliver, M., and Bissett, P. (2005). Harmful Algal Blooms in a Dynamic Environment: How Can Optics Help The Field-Going and Sample-Poor Biologist? UNESCO Monographs on Oceanographic Methodology- Manual on Harmful Marine Microalgae, UNESCO [submitted, refereed].

Bissett, W.P., Arnone, R., DeBra, S., Deterlie, D., Dye, D., Kirkpatrick, G., Schofield, O. and Walsh, J. (2005). Predicting the Inherent Optical Properties and Colored Dissolved Organic Matter Dynamics on the West Florida Shelf. Marine Chemistry, 95, 199-233, [published, refereed].

Glenn, S., Arnone, R., Bergman, T., Bissett, P., Crowley, M., Cullen, J., Gryzmski, J., Haidvogel, D., Kohut, J., Moline, M., Oliver, M., Orrico, C., Sherrell, R., Song, T., Weidemann, A., Chant, R. and Schofield, O., 2004. The Biogeochemical Impact of Summertime Coastal Upwelling on the New Jersey Shelf. Journal of Geophysical Research: 109 (C12S04), [published, refereed].

Chen, R.F., Bissett, W.P., Coble, P., Conmy, R., G. Gardner, B., Moran, M.A., Wang, X., Wells, M.L., Whelan, P. and Zepp, R.G. (2004). Chromophoric Dissolved Organic Matter (CDOM) Source Characterization in the Louisiana Bight. Marine Chemistry, 89(1-4): 257-272, [published, refereed].

Kohler, D.D.R., Bissett, W.P., Steward, R.G. and Davis, C.O., 2004. A New Approach for the Radiometric Calibration of Spectral Imaging Systems. Optics Express, 12(11), [published, refereed].

Mobley, C.D., Stramski, D., Bissett, W.P. and Boss, E., 2004. Optical modeling of ocean waters: Is the Case 1 - Case 2 classification still useful? Oceanography, 17(2): 60-67, [published, refereed].

Oliver, M.J., Kohut, J.T., Irwin, A.J.G., Schofield, O.M., Glenn, S., Moline, M.A., and Bissett, W.P. (2004). Bioinformatic Approaches for Objective Detection of Water Masses. Journal of Geophysical Research, 109(C7): 12, [published, refereed].

Philpot, W.D., Davis, C.O., Bissett, W.P., Mobley, C., Kohler, D.D.R., Lee, Z.P., Snyder, W., Steward, R.G., Gould, R. and Arnone, R., 2004. Bottom characterization from hyperspectral image data. Oceanography, 17(2): 76-85, [published, refereed].

Schofield, O., Arnone, R., Bissett, P., Dickey, T., Davis, C., Finkel, Z., Oliver, M. and Moline, M., 2004. Watercolors in the coastal zone: what can we see? Oceanography, 17(2): 24-31, [published, refereed].

Schofield, O., Bergmann, T., Oliver, M., Moline, M., and Bissett, P. (2004). Inversion of the Bulk Absorption in the Mid-Atlantic Bight and its Utility for Water Mass Analysis in Optically Complex Coastal Waters. Journal of Geophysical Research, 190(C12S04): 12 [published, refereed].

Schofield, O., Bissett, W. P., Frazer, T.K., Iglesias-Rodriguez, D., Moline, M.A., Glenn, S. (2003). Development of Regional Coastal Ocean Observatories and the Potential Benefits to Marine Sanctuaries, Marine Technology Society Journal, 37 (1): 54-67, [published, refereed].

Shulman, I., Haddock, S.H.D., McGillicuddy, D.J.Jr., D. Paduan, J.D., Bissett, W.P. (2003). Numerical Modeling of Bioluminescence Distributions in the Coastal Ocean. Journal of Atmospheric and Oceanic Technology 20 (7):1060-1068, [published, refereed].

Zhang, X., Lewis, M., Bissett, P. and Johnson, B. (2004) Optical Influence of Ship Wakes. Applied Optics, 43(15): 3122-3132, [published, refereed].

Davis, C. O., Bissett, W. P., Brown, C. (2003). Optical remote sensing of the coastal ocean: Future directions for observing and monitoring, Earth System Monitor, Vol. 13, No. 2, [published].

Davis, C. O., J. Bowles, R. A. Leathers, D. Korwan, T. V. Downes, W. A. Snyder, W. J. Rhea, W. Chen, J. Fisher, W. P. Bissett and R. A. Reisse (2002). Ocean PHILLS hyperspectral imager: design, characterization, and calibration, Optics Express, 10(4): 210-221, [published, refereed].

Schofield, O., Bergmann, T., Bissett, W. P., Grassle, F., Haidvogel, D., Kohut, J., Moline, M., Glenn, S. (2002). Linking regional coastal observatories to provide the foundation for a national ocean observation network. Journal of Oceanic Engineering, 27(2): 146-154, [published, refereed].

Schofield, O., Glenn, S., Chant, R., Moline, M. A., Bissett, P., Haidvogel, D., and Wilkins, J. (2002). The evolution of a nearshore coastal observatory and the establishment of the New Jersey Shelf Observing System. Oceanology International 2002, [published].

Walsh J.J., Haddad, K.D., Dieterle, D.A., Weisberg, R.H., Li, Z., Yang, H., Muller-Karger, F.E., Heil, C.A., and Bissett, W.P., (2002). A numerical analysis of landfall of the 1979 red tide of Karenia brevis along the west coast of Florida. Continental Shelf Research, 22(1):15-38, [published, refereed].

Bissett, W. P, Schofield, O., Glenn, S., Cullen, J. J., Miller, W. L., Plueddemann, A. J., Mobley, C. D., (2001). Resolving the impacts and feedbacks of ocean optics on upper ocean ecology. Oceanography, 14:30-49, [published, refereed].

Walsh, J.J., B. Penta, D.A. Dieterle, and W. P. Bissett. (2001). Predictive ecological modeling of harmful algal blooms. Human Ecological Risk Assessment, 7:1369-1383, [published, refereed].

Bissett, W.P., Schofield, O., Mobley, C., Crowley, M.F., and Moline, M.A. (2000). Optical Remote Sensing Techniques in Biological Oceanography. Methods in Microbiology, Volume 30: Marine Microbiology (J.H. Paul, ed), Academic Press, London. 519-540, [published, refereed].

Bissett, W. P., J. J. Walsh, D. A. Dieterle and K. L. Carder (1999). Carbon cycling in the upper waters of the Sargasso Sea: I. Numerical simulation of differential carbon and nitrogen fluxes. Deep-Sea Research, 46(2):205-269, [published, refereed].

Bissett, W. P., K. L. Carder, J. J. Walsh and D. A. Dieterle (1999). Carbon cycling in the upper waters of the Sargasso Sea: II. Numerical simulation of apparent and inherent optical properties. Deep-Sea Research, 46(2):271-317, [published, refereed].

Schofield, O., Grzymski, J., Bissett, W.P., Kirkpatrick, G., Millie, D.F., Moline, M., and Roesler, C.S. (1999). Optical monitoring and forecasting systems for harmful algal blooms: possibility or pipe dream? Journal of Phycology, 35, 1477-1496, [published, refereed].

Walsh, J.J., D. A. Dieterle, F. E. Muller-Karger, R. Bohrer, W. P. Bissett, R. J. Varela, R. Aparicio, R. Diaz, R. Thunell, G. T. Taylor, M. I. Scranton, K. A. Fanning, and E. T. Peltzer (1999). Simulation of carbon-nitrogen cycling during spring upwelling in the Cariaco Basin. Journal of Geophysical Research, 104, 7807-7825, [published, refereed].

HONORS/AWARDS/PRIZES

Semi-Finalist, 2003 Small Business of the Year, Florida Environmental Research Institute, W. Paul Bissett, Ph.D., Executive Director, Greater Tampa Chamber of Commerce.

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